



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:30 AM GMT

PDB ID : 3CEM  
Title : Human glycogen phosphorylase (tense state) in complex with the allosteric inhibitor AVE9423  
Authors : Wendt, K.U.; Dreyer, M.K.; Anderka, O.; Klabunde, T.; Loenze, P.; Defossa, E.; Schmoll, D.  
Deposited on : 2008-02-29  
Resolution : 2.47 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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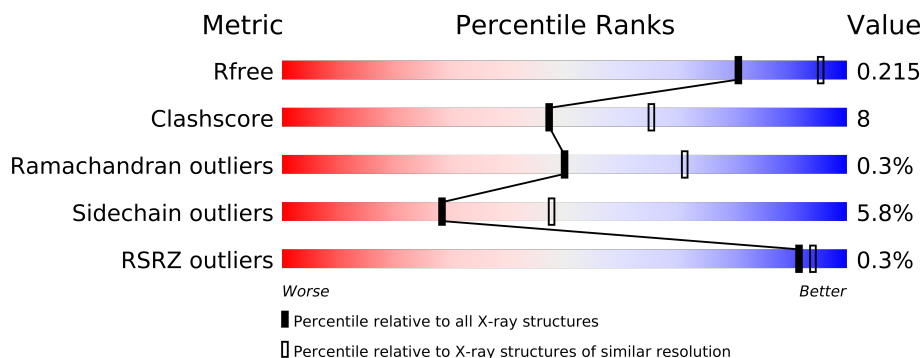
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	3277 (2.50-2.46)
Clashscore	79885	4136 (2.50-2.46)
Ramachandran outliers	78287	4052 (2.50-2.46)
Sidechain outliers	78261	4054 (2.50-2.46)
RSRZ outliers	66119	3279 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	809	
1	B	809	

## 2 Entry composition i

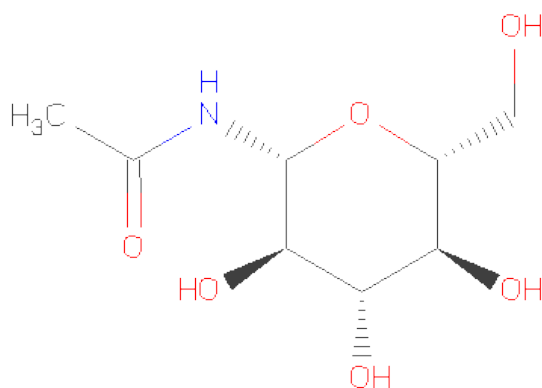
There are 5 unique types of molecules in this entry. The entry contains 13570 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

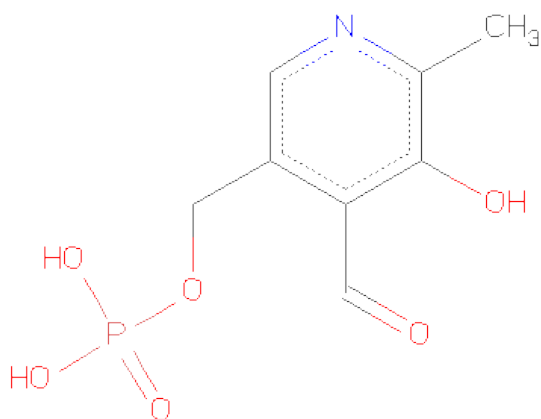
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	794	Total	C	N	O	S	0	1	0
			6460	4150	1097	1184	29			
1	B	794	Total	C	N	O	S	0	3	0
			6479	4161	1101	1188	29			

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



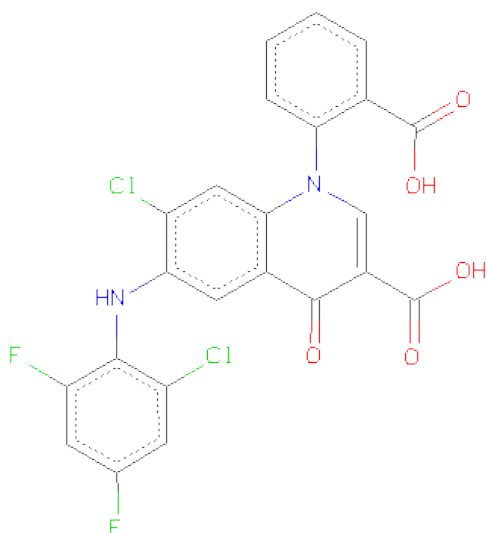
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 4 is 1-(2-CARBOXYPHENYL)-7-CHLORO-6-[(2-CHLORO-4,6-DIFLUOROPHENYL)AMINO]-4-OXO-1,4-DIHYDROQUINOLINE-3-CARBOXYLICACID (three-letter code: AVD) (formula:  $C_{23}H_{12}Cl_2F_2N_2O_5$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			34	23	2	2	2	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O	0	0
			34	23	2	2	2	5		

- Molecule 5 is water.

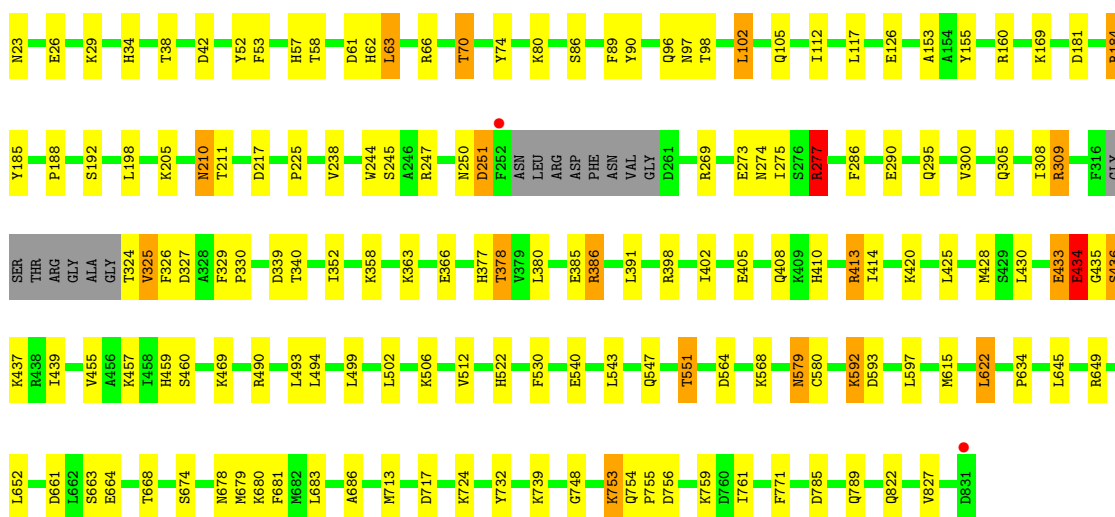
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	274	Total	O	0	0
			274	274		
5	B	227	Total	O	0	0
			227	227		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

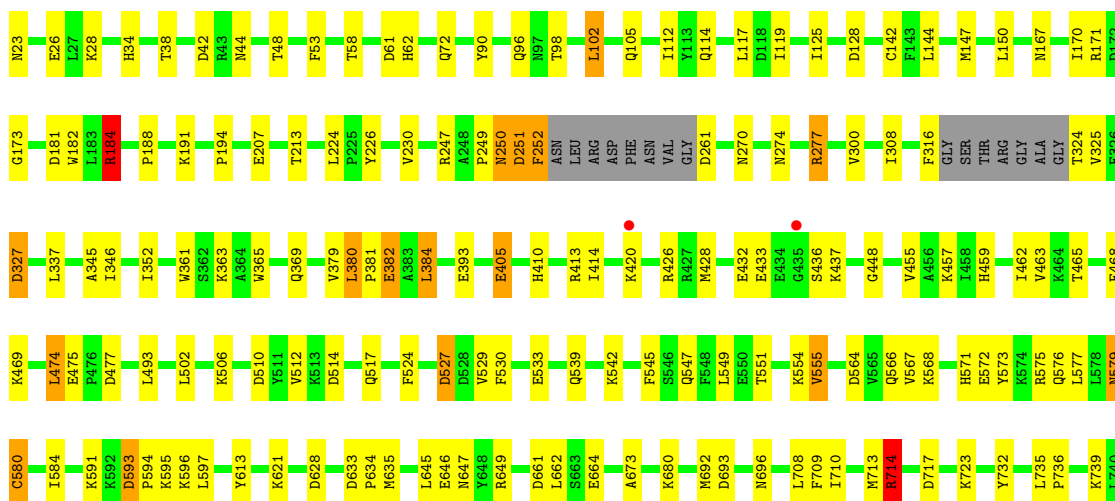
- Molecule 1: Glycogen phosphorylase, liver form

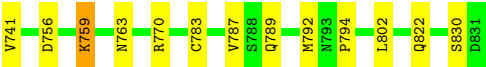
Chain A:



- Molecule 1: Glycogen phosphorylase, liver form

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.38Å 124.38Å 123.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.39 – 2.47 49.36 – 2.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.39-2.47) 99.9 (49.36-2.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.155 , 0.215 0.156 , 0.215	Depositor DCC
$R_{free}$ test set	5343 reflections (7.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 16.5	EDS
Estimated twinning fraction	0.029 for -h,-k,l 0.095 for h,-h-k,-l 0.037 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 76582 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AVD, NBG, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.97	2/6605 (0.0%)	0.92	10/8931 (0.1%)
1	B	0.94	3/6625 (0.0%)	0.92	14/8958 (0.2%)
All	All	0.95	5/13230 (0.0%)	0.92	24/17889 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	GLU	CG-CD	5.71	1.60	1.51
1	B	182	TRP	CE3-CZ3	5.24	1.47	1.38
1	A	405	GLU	CG-CD	5.21	1.59	1.51
1	B	142	CYS	CB-SG	5.21	1.91	1.82
1	B	580	CYS	CB-SG	-5.13	1.73	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	490	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	514	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	770	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	B	171	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	B	575	ARG	NE-CZ-NH2	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	ARG	CA-CB-CG	6.36	127.38	113.40
1	B	184	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	649	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	575	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	192	SER	N-CA-CB	-6.06	101.41	110.50
1	B	714	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	474	LEU	CA-CB-CG	5.97	129.02	115.30
1	A	277	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	661	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	A	160	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	714	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	514	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	A	377	HIS	CB-CA-C	-5.28	99.85	110.40
1	B	770	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	309	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	430	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	380	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	B	708	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	249	PRO	Peptide
1	B	250	ASN	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6460	0	6447	106	0
1	B	6479	0	6458	108	0
2	A	15	0	15	0	0
2	B	15	0	14	0	0
3	A	16	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	7	2	0
4	A	34	0	10	0	0
4	B	34	0	10	0	0
5	A	274	0	0	17	0
5	B	227	0	0	13	0
All	All	13570	0	12968	208	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (208) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:547:GLN:O	1:A:551:THR:HG23	1.57	1.02
1:B:250:ASN:HA	1:B:251:ASP:OD2	1.61	1.00
1:B:96:GLN:HE21	1:B:105:GLN:HE22	0.94	0.94
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.53	0.90
1:B:361:TRP:CH2	1:B:405:GLU:HG2	2.06	0.90
1:A:66:ARG:O	1:A:70:THR:HG23	1.72	0.89
1:A:305:GLN:HG3	5:A:863:HOH:O	1.74	0.85
1:B:274:ASN:ND2	1:B:277:ARG:HH11	1.74	0.85
1:B:96:GLN:HE21	1:B:105:GLN:NE2	1.76	0.83
1:A:184:ARG:HH11	1:A:184:ARG:HG3	1.44	0.81
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.26	0.81
1:A:198:LEU:HD22	1:A:305:GLN:NE2	1.95	0.81
1:B:251:ASP:HB3	1:B:252:PHE:HA	1.62	0.81
1:B:96:GLN:NE2	1:B:105:GLN:HE22	1.79	0.79
1:B:714:ARG:HG2	1:B:714:ARG:HH11	1.48	0.78
1:B:756:ASP:HB2	5:B:1031:HOH:O	1.84	0.78
1:A:290:GLU:HG3	1:A:391:LEU:HD11	1.66	0.78
1:A:66:ARG:O	1:A:70:THR:CG2	2.32	0.77
1:A:634:PRO:HA	5:A:905:HOH:O	1.86	0.75
1:B:830:SER:HB3	5:B:1019:HOH:O	1.87	0.74
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.71	0.73
1:A:70:THR:HG21	1:A:238:VAL:H	1.52	0.73
1:A:324:THR:N	1:A:325:VAL:HB	2.04	0.72
1:A:251:ASP:OD1	1:A:251:ASP:N	2.23	0.72
1:B:274:ASN:HD22	1:B:277:ARG:HH11	1.35	0.71
1:A:386:ARG:HH11	1:A:386:ARG:HB2	1.56	0.70
1:A:274:ASN:ND2	1:A:277:ARG:HH11	1.91	0.69
1:B:251:ASP:CB	1:B:252:PHE:HA	2.22	0.68
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.74	0.68
3:B:832:PLP:H5A1	3:B:832:PLP:O4A	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:455:VAL:H	1:B:459:HIS:HD2	1.43	0.67
1:A:184:ARG:NH2	1:B:250:ASN:HB3	2.10	0.66
1:A:324:THR:HA	1:A:326:PHE:H	1.58	0.66
1:B:436:SER:O	1:B:437:LYS:HB2	1.94	0.66
1:A:615:MET:CE	1:A:761:ILE:HG12	2.25	0.66
1:A:80:LYS:HB3	1:A:827:VAL:HG12	1.78	0.65
1:B:527:ASP:OD2	1:B:529:VAL:HB	1.97	0.64
1:A:437:LYS:HD2	5:A:1057:HOH:O	1.97	0.64
1:A:184:ARG:NH1	1:A:184:ARG:HG3	2.12	0.64
1:B:547:GLN:O	1:B:551:THR:HG23	1.97	0.64
1:B:633:ASP:OD2	1:B:635:MET:HB2	1.99	0.63
1:B:181:ASP:OD2	1:B:184:ARG:HG3	1.97	0.63
1:A:181:ASP:OD2	1:A:184:ARG:NH1	2.32	0.62
1:B:250:ASN:CA	1:B:251:ASP:OD2	2.43	0.62
1:B:224:LEU:HD23	1:B:247[A]:ARG:HE	1.65	0.62
1:B:436:SER:HA	5:B:1028:HOH:O	1.99	0.62
1:B:477:ASP:HB2	5:B:901:HOH:O	2.00	0.61
1:B:324:THR:HA	1:B:327:ASP:OD1	2.01	0.61
1:B:584:ILE:HG22	1:B:741:VAL:HG22	1.82	0.61
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.84	0.61
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.83	0.61
1:A:274:ASN:HD22	1:A:277:ARG:HH11	1.49	0.60
1:B:591:LYS:NZ	1:B:635:MET:HG3	2.15	0.60
1:B:361:TRP:CZ3	1:B:405:GLU:HG2	2.36	0.60
1:B:662:LEU:HD22	1:B:787:VAL:HG11	1.84	0.60
1:B:542:LYS:NZ	1:B:661:ASP:OD2	2.26	0.60
1:B:316:PHE:C	5:B:971:HOH:O	2.40	0.60
1:A:184:ARG:HD2	1:A:185:TYR:CZ	2.38	0.59
1:B:207:GLU:HG3	5:B:859:HOH:O	2.03	0.59
1:A:597:LEU:HA	5:A:984:HOH:O	2.03	0.59
1:B:274:ASN:HD22	1:B:277:ARG:HD2	1.67	0.59
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.84	0.59
1:A:29:LYS:HE2	5:A:1046:HOH:O	2.02	0.58
1:A:592:LYS:HD2	1:A:592:LYS:O	2.04	0.58
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.39	0.58
1:B:226:TYR:OH	1:B:247[A]:ARG:NH2	2.37	0.57
1:B:23:ASN:HD22	1:B:26[A]:GLU:HG2	1.69	0.56
1:B:42:ASP:HB3	5:B:1056:HOH:O	2.04	0.56
1:A:274:ASN:HD22	1:A:277:ARG:HD2	1.71	0.56
1:B:759:LYS:O	1:B:763:ASN:HB2	2.06	0.56
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.41	0.55
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:785:ASP:O	1:A:789:GLN:HG3	2.06	0.54
1:B:714:ARG:CG	1:B:714:ARG:HH11	2.17	0.54
1:A:522:HIS:CD2	5:A:860:HOH:O	2.60	0.54
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.91	0.54
1:A:580:CYS:SG	1:A:622:LEU:HD13	2.48	0.53
1:A:339:ASP:OD1	1:A:340:THR:N	2.38	0.53
1:A:184:ARG:HA	1:B:247[B]:ARG:NH1	2.24	0.53
1:A:42:ASP:HB2	5:A:910:HOH:O	2.07	0.53
1:A:398:ARG:O	1:A:402:ILE:HG13	2.09	0.53
5:A:1016:HOH:O	1:B:250:ASN:HB3	2.08	0.53
1:B:579:ASN:HD22	1:B:579:ASN:C	2.12	0.53
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.90	0.52
1:A:247[B]:ARG:NH2	1:B:184:ARG:HG2	2.25	0.52
1:B:48:THR:HG22	1:B:125:ILE:HG13	1.92	0.52
1:A:275:ILE:O	1:A:295:GLN:HG2	2.09	0.52
1:B:554:LYS:HG3	1:B:555:VAL:H	1.75	0.51
1:B:591:LYS:HZ2	1:B:635:MET:HG3	1.74	0.51
1:A:455:VAL:H	1:A:459:HIS:HD2	1.59	0.51
1:B:261:ASP:HB3	5:B:1058:HOH:O	2.10	0.51
1:B:361:TRP:CH2	1:B:405:GLU:CG	2.87	0.51
1:A:420:LYS:HG2	1:A:420:LYS:O	2.11	0.51
1:A:414:ILE:HG22	1:A:425:LEU:HD23	1.93	0.51
1:A:74:TYR:CZ	1:A:153:ALA:HA	2.46	0.50
1:A:680:LYS:NZ	3:A:832:PLP:O3	2.43	0.50
5:A:1016:HOH:O	1:B:250:ASN:CB	2.60	0.50
1:A:408:GLN:HG3	5:A:1064:HOH:O	2.12	0.49
1:A:324:THR:N	1:A:325:VAL:CB	2.73	0.49
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.95	0.49
1:B:692:MET:HG2	1:B:710:ILE:HG21	1.94	0.49
1:A:185:TYR:CD2	1:B:194:PRO:HB3	2.48	0.49
1:A:410:HIS:HD2	1:A:413:ARG:HH11	1.60	0.49
1:A:678:ASN:OD1	1:A:679:MET:N	2.45	0.49
1:A:436:SER:HB3	5:A:990:HOH:O	2.12	0.49
1:A:386:ARG:NH1	1:A:386:ARG:HB2	2.26	0.48
1:B:112:ILE:HG13	1:B:119:ILE:HD13	1.95	0.48
1:A:506:LYS:HG3	1:A:530:PHE:CE1	2.48	0.48
1:A:211:THR:O	1:A:358:LYS:NZ	2.46	0.48
1:B:530:PHE:HE2	1:B:802:LEU:HD13	1.79	0.48
1:A:53:PHE:HE1	1:A:188:PRO:HD3	1.78	0.48
1:B:593:ASP:C	1:B:595:LYS:H	2.15	0.48
1:B:173:GLY:HA3	5:B:963:HOH:O	2.13	0.48
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:732:TYR:CE1	1:B:739:LYS:HG3	2.49	0.47
1:B:680:LYS:NZ	3:B:832:PLP:O3	2.47	0.47
1:B:506:LYS:HB3	1:B:524:PHE:CZ	2.49	0.47
1:B:510:ASP:HB3	1:B:517:GLN:OE1	2.15	0.47
1:A:324:THR:HG21	5:A:1021:HOH:O	2.14	0.47
1:A:386:ARG:HA	1:A:439:ILE:O	2.15	0.47
1:B:381:PRO:HA	1:B:384:LEU:HD22	1.96	0.47
1:A:753:LYS:O	1:A:754:GLN:HG3	2.14	0.47
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.97	0.47
1:B:571[A]:HIS:ND1	1:B:572:GLU:N	2.62	0.47
1:B:379:VAL:CG2	1:B:673:ALA:HB2	2.45	0.47
1:B:380:LEU:HG	1:B:382:GLU:OE2	2.15	0.47
1:A:460:SER:HB2	5:A:1042:HOH:O	2.15	0.47
1:B:477:ASP:N	5:B:901:HOH:O	2.47	0.46
1:A:436:SER:HA	5:A:1018:HOH:O	2.15	0.46
1:B:539:GLN:OE1	1:B:539:GLN:HA	2.16	0.46
1:A:668:THR:OG1	1:A:771:PHE:HB3	2.15	0.46
1:A:198:LEU:HD13	1:A:305:GLN:HB3	1.96	0.46
1:A:732:TYR:O	1:A:739:LYS:HB2	2.16	0.46
1:A:410:HIS:HE1	1:A:428:MET:O	1.98	0.46
1:A:681:PHE:HB3	1:A:686:ALA:HB3	1.98	0.46
1:A:58:THR:O	1:A:62:HIS:HD2	1.98	0.46
1:A:579:ASN:C	1:A:579:ASN:HD22	2.20	0.46
1:A:184:ARG:HH21	1:B:250:ASN:HB3	1.81	0.46
1:A:494:LEU:HD23	1:A:494:LEU:C	2.37	0.45
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.56	0.45
1:A:210:ASN:C	1:A:210:ASN:HD22	2.19	0.45
1:A:57:HIS:HD2	5:A:1030:HOH:O	1.98	0.45
1:B:58:THR:O	1:B:62:HIS:HD2	1.99	0.45
1:A:378:THR:HB	5:A:1061:HOH:O	2.16	0.45
1:B:26[B]:GLU:OE1	1:B:62:HIS:HE1	2.00	0.45
1:B:593:ASP:O	1:B:595:LYS:N	2.50	0.45
1:A:547:GLN:O	1:A:551:THR:CG2	2.46	0.45
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.52	0.44
1:B:564:ASP:OD1	1:B:664:GLU:OE2	2.35	0.44
1:B:465:THR:O	1:B:469:LYS:HD3	2.16	0.44
1:B:432:GLU:O	1:B:437:LYS:HA	2.17	0.44
1:A:63:LEU:HD12	1:A:63:LEU:C	2.37	0.44
1:A:96:GLN:NE2	1:A:105:GLN:HE22	2.06	0.44
1:B:28:LYS:HE2	1:B:114:GLN:NE2	2.32	0.44
1:A:564:ASP:OD1	1:A:664:GLU:OE2	2.35	0.43
1:B:144:LEU:HD23	1:B:147:MET:CE	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.00	0.43
1:A:649:ARG:HH11	1:A:649:ARG:HG2	1.82	0.43
1:A:410:HIS:HD2	1:A:413:ARG:NH1	2.16	0.43
1:B:732:TYR:CZ	1:B:739:LYS:HG3	2.52	0.43
1:B:635:MET:HA	5:B:992:HOH:O	2.18	0.43
1:B:365:TRP:CD1	1:B:369:GLN:NE2	2.86	0.43
1:A:756:ASP:O	1:A:759:LYS:HB2	2.18	0.43
1:A:86:SER:HB3	1:A:89:PHE:CE1	2.54	0.43
1:B:735:LEU:HA	1:B:736:PRO:HD2	1.72	0.43
1:A:184:ARG:CG	1:A:184:ARG:HH11	2.19	0.42
1:B:577:LEU:O	1:B:580:CYS:HB3	2.18	0.42
1:B:693:ASP:O	1:B:696:ASN:HB2	2.18	0.42
1:A:205:LYS:HB3	1:A:205:LYS:HE2	1.86	0.42
1:B:596:LYS:HG2	1:B:597:LEU:N	2.34	0.42
1:B:545:PHE:CE2	1:B:549:LEU:HD11	2.53	0.42
1:A:250:ASN:ND2	1:A:269:ARG:HH22	2.18	0.42
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.55	0.42
1:B:98:THR:HG22	1:B:102:LEU:HD22	2.02	0.42
1:A:184:ARG:HH22	1:B:250:ASN:HB3	1.85	0.42
1:B:112:ILE:HG23	1:B:117:LEU:HB2	2.02	0.42
1:A:247[B]:ARG:HA	1:A:273:GLU:HG2	2.01	0.42
1:A:23:ASN:ND2	1:A:26:GLU:HG2	2.35	0.42
1:A:98:THR:HG22	1:A:102:LEU:HD22	2.02	0.41
1:B:593:ASP:N	1:B:594:PRO:HD3	2.35	0.41
1:B:270:ASN:ND2	5:B:972:HOH:O	2.52	0.41
1:B:633:ASP:HA	1:B:634:PRO:HD3	1.78	0.41
1:B:463:VAL:HG13	1:B:468:PHE:CD1	2.55	0.41
1:A:748:GLY:HA3	1:A:755:PRO:HA	2.02	0.41
1:A:80:LYS:HE3	1:A:330:PRO:O	2.21	0.41
1:B:167:ASN:HD22	1:B:647:ASN:HD21	1.68	0.41
1:A:250:ASN:OD1	1:B:184:ARG:NH2	2.53	0.41
1:B:414:ILE:HD13	1:B:428:MET:SD	2.59	0.41
1:B:363:LYS:O	1:B:363:LYS:HD3	2.20	0.41
1:A:198:LEU:HA	1:A:198:LEU:HD23	1.84	0.41
1:A:753:LYS:HD2	1:A:753:LYS:HA	1.99	0.41
1:A:493:LEU:HD21	1:A:512:VAL:HG22	2.03	0.41
1:A:66:ARG:O	1:A:70:THR:HG22	2.18	0.41
1:B:493:LEU:HD11	1:B:512:VAL:HG22	2.03	0.41
1:B:792:MET:O	1:B:794:PRO:HD3	2.20	0.41
1:B:567:VAL:O	1:B:568:LYS:HB3	2.21	0.40
1:B:42:ASP:HB2	5:B:886:HOH:O	2.20	0.40
1:B:530:PHE:HA	1:B:533:GLU:OE2	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:LEU:HB3	1:B:230:VAL:HG11	2.04	0.40
1:A:97:ASN:ND2	5:A:891:HOH:O	2.54	0.40
1:A:433:GLU:O	1:A:434:GLU:O	2.38	0.40
1:A:52:TYR:CZ	1:A:126:GLU:HB2	2.56	0.40
1:A:112:ILE:HG23	1:A:117:LEU:HB2	2.04	0.40
1:B:308:ILE:HD13	1:B:352:ILE:HG21	2.01	0.40
1:B:53:PHE:HE1	1:B:188:PRO:HD3	1.86	0.40
1:A:329:PHE:HB3	1:A:330:PRO:HD3	2.04	0.40
1:A:663:SER:HB2	1:A:681:PHE:CG	2.56	0.40
1:B:410:HIS:HE1	1:B:428:MET:O	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/809 (98%)	749 (95%)	37 (5%)	3 (0%)	43	64
1	B	791/809 (98%)	750 (95%)	39 (5%)	2 (0%)	50	71
All	All	1580/1618 (98%)	1499 (95%)	76 (5%)	5 (0%)	50	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	B	555	VAL
1	B	527	ASP
1	A	593	ASP
1	A	435	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of



similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	697/706 (99%)	656 (94%)	41 (6%)	28	46
1	B	699/706 (99%)	659 (94%)	40 (6%)	29	48
All	All	1396/1412 (99%)	1315 (94%)	81 (6%)	28	48

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	70	THR
1	A	90	TYR
1	A	102	LEU
1	A	155	TYR
1	A	169	LYS
1	A	184	ARG
1	A	210	ASN
1	A	217	ASP
1	A	245	SER
1	A	251	ASP
1	A	277	ARG
1	A	300	VAL
1	A	309	ARG
1	A	325	VAL
1	A	327	ASP
1	A	363	LYS
1	A	378	THR
1	A	380	LEU
1	A	386	ARG
1	A	413	ARG
1	A	433	GLU
1	A	434	GLU
1	A	436	SER
1	A	457	LYS
1	A	469	LYS
1	A	499	LEU
1	A	502	LEU
1	A	540	GLU
1	A	543	LEU
1	A	551	THR
1	A	568	LYS
1	A	579	ASN

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Mol	Chain	Res	Type
1	A	592	LYS
1	A	622	LEU
1	A	645	LEU
1	A	652	LEU
1	A	683	LEU
1	A	724	LYS
1	A	753	LYS
1	A	822	GLN
1	B	44	ASN
1	B	72	GLN
1	B	90	TYR
1	B	102	LEU
1	B	128	ASP
1	B	150	LEU
1	B	184	ARG
1	B	191	LYS
1	B	213	THR
1	B	251	ASP
1	B	252	PHE
1	B	277	ARG
1	B	325	VAL
1	B	327	ASP
1	B	337	LEU
1	B	382	GLU
1	B	384	LEU
1	B	393	GLU
1	B	405	GLU
1	B	413	ARG
1	B	420	LYS
1	B	426	ARG
1	B	433	GLU
1	B	457	LYS
1	B	462	ILE
1	B	474	LEU
1	B	475	GLU
1	B	502	LEU
1	B	573	TYR
1	B	579	ASN
1	B	593	ASP
1	B	613	TYR
1	B	621	LYS
1	B	628	ASP

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Mol	Chain	Res	Type
1	B	645	LEU
1	B	714	ARG
1	B	723	LYS
1	B	759	LYS
1	B	789	GLN
1	B	822	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	32	ASN
1	A	34	HIS
1	A	57	HIS
1	A	62	HIS
1	A	96	GLN
1	A	97	ASN
1	A	114	GLN
1	A	167	ASN
1	A	208	HIS
1	A	210	ASN
1	A	239	ASN
1	A	250	ASN
1	A	270	ASN
1	A	274	ASN
1	A	305	GLN
1	A	410	HIS
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	539	GLN
1	A	541	ASN
1	A	566	GLN
1	A	579	ASN
1	A	768	HIS
1	A	822	GLN
1	B	23	ASN
1	B	34	HIS
1	B	57	HIS
1	B	62	HIS
1	B	105	GLN
1	B	114	GLN

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Mol	Chain	Res	Type
1	B	167	ASN
1	B	239	ASN
1	B	270	ASN
1	B	274	ASN
1	B	305	GLN
1	B	369	GLN
1	B	410	HIS
1	B	443	HIS
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN
1	B	566	GLN
1	B	579	ASN
1	B	789	GLN
1	B	822	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NBG	A	1	-	15,15,15	1.60	3 (20%)	21,21,21	1.12	2 (9%)
3	PLP	A	832	1	16,16,16	1.21	1 (6%)	23,23,23	1.00	3 (13%)
4	AVD	A	833	-	37,37,37	1.13	3 (8%)	52,55,55	1.62	9 (17%)
2	NBG	B	2	-	15,15,15	1.62	3 (20%)	21,21,21	1.88	5 (23%)
3	PLP	B	832	1	16,16,16	1.21	1 (6%)	23,23,23	1.01	3 (13%)
4	AVD	B	833	-	37,37,37	1.57	8 (21%)	52,55,55	1.82	15 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NBG	A	1	-	-	0/5/26/26	0/1/1/1
3	PLP	A	832	1	-	0/8/8/8	0/1/1/1
4	AVD	A	833	-	-	0/16/16/16	0/2/4/4
2	NBG	B	2	-	-	0/5/26/26	0/1/1/1
3	PLP	B	832	1	-	0/8/8/8	0/1/1/1
4	AVD	B	833	-	-	0/16/16/16	0/2/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	833	AVD	C23-C26	4.22	1.58	1.50
4	B	833	AVD	C22-N21	3.90	1.40	1.35
2	A	1	NBG	O5-C1	-3.23	1.39	1.44
2	B	2	NBG	O5-C1	-2.87	1.39	1.44
4	B	833	AVD	C34-C39	2.74	1.55	1.49
2	B	2	NBG	O3-C3	-2.59	1.36	1.43
4	B	833	AVD	C16-N21	2.58	1.45	1.40
4	A	833	AVD	C23-C26	2.53	1.55	1.50
3	B	832	PLP	C2-N1	2.50	1.38	1.33
3	A	832	PLP	C2-N1	2.46	1.38	1.33
2	A	1	NBG	C2-C1	-2.35	1.50	1.52
2	B	2	NBG	O5-C5	-2.25	1.38	1.44
4	A	833	AVD	C34-C39	2.23	1.54	1.49
4	B	833	AVD	C6-C1	2.21	1.41	1.37
4	A	833	AVD	F11-C5	-2.16	1.31	1.36
4	B	833	AVD	C6-C5	2.14	1.41	1.37
4	B	833	AVD	C15-C14	2.10	1.39	1.36
2	A	1	NBG	O5-C5	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	833	AVD	F11-C5	-2.03	1.31	1.36

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	833	AVD	C15-C14-CL29	-5.73	114.77	119.16
4	A	833	AVD	C30-C28-N21	5.15	123.93	118.27
2	B	2	NBG	O2-C2-C3	-4.39	100.50	110.35
4	A	833	AVD	C15-C14-CL29	-3.85	116.21	119.16
4	B	833	AVD	C30-C28-N21	3.77	122.41	118.27
4	B	833	AVD	O27-C26-C23	3.38	124.07	114.37
2	B	2	NBG	C1-N1-C7	3.29	126.05	122.44
2	A	1	NBG	O2-C2-C1	-3.10	103.49	109.30
4	A	833	AVD	C28-N21-C16	3.08	123.43	120.15
2	B	2	NBG	O5-C1-C2	-2.98	107.02	109.70
4	B	833	AVD	C14-C15-C16	2.97	122.05	117.39
4	B	833	AVD	C18-C13-C14	-2.86	114.66	117.99
4	A	833	AVD	C33-C34-C28	2.84	121.73	118.61
4	B	833	AVD	O42-C26-C23	-2.73	115.11	122.18
4	B	833	AVD	F9-C1-C2	2.70	120.03	117.73
4	B	833	AVD	C6-C1-C2	-2.69	120.69	123.59
4	B	833	AVD	C13-C14-CL29	2.67	123.00	119.45
2	B	2	NBG	C2-C1-N1	-2.64	107.87	111.44
4	B	833	AVD	C15-C16-C17	-2.62	116.50	120.68
4	A	833	AVD	C28-C34-C39	-2.52	120.36	123.69
2	A	1	NBG	O5-C1-C2	2.51	111.96	109.70
2	B	2	NBG	C3-C4-C5	-2.48	105.77	110.20
3	B	832	PLP	O4A-C4A-C4	-2.47	119.99	125.32
3	A	832	PLP	O4A-C4A-C4	-2.45	120.03	125.32
4	A	833	AVD	C18-C17-C16	2.43	122.33	118.64
4	B	833	AVD	C14-C13-N10	2.32	123.54	119.47
4	B	833	AVD	C22-N21-C28	2.25	121.39	118.52
3	B	832	PLP	C3-C4-C5	2.16	119.85	118.15
3	A	832	PLP	C5-C6-N1	-2.10	120.08	123.86
4	A	833	AVD	C6-C1-C2	-2.09	121.33	123.59
3	B	832	PLP	C5-C6-N1	-2.08	120.10	123.86
4	A	833	AVD	C3-C4-C5	-2.08	116.28	117.75
4	B	833	AVD	C1-C2-N10	-2.05	119.37	122.12
4	B	833	AVD	C13-C18-C17	2.05	123.25	120.81
4	A	833	AVD	C17-C16-N21	2.04	121.62	117.79
4	B	833	AVD	C22-N21-C16	-2.02	117.44	121.32
3	A	832	PLP	C3-C4-C5	2.01	119.73	118.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	794/809 (98%)	-0.55	2 (0%) 91 94	18, 32, 56, 72	0
1	B	794/809 (98%)	-0.51	2 (0%) 91 94	16, 34, 61, 75	0
All	All	1588/1618 (98%)	-0.53	4 (0%) 91 94	16, 33, 59, 75	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	PHE	3.2
1	B	435	GLY	2.5
1	B	420	LYS	2.4
1	A	831	ASP	2.4

### 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PLP	B	832	16/16	0.14	1.89	19,25,32,33	0
3	PLP	A	832	16/16	0.14	1.58	18,23,33,34	0
4	AVD	A	833	34/34	0.11	-0.21	22,28,37,42	0
4	AVD	B	833	34/34	0.11	-0.37	20,29,32,36	0
2	NBG	A	1	15/15	0.10	-0.68	18,26,33,33	0
2	NBG	B	2	15/15	0.09	-1.01	22,27,33,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.